ALGORITHM DEVELOPMENT AND SPECTROSCOPIC MODELING FOR SPACE WEATHER APPLICATIONS

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LONG-TERM GOAL

The focus of our research is the global remote sensing of the ionosphere via ultraviolet emissions observed from space. We are developing optimal methods for inverting satellite-based measurements using nonlinear techniques. One aspect of this work involves understanding the effects of latitude gradients and including these in the inversion algorithm. Another primary concern is development of rigorous error estimation techniques.

A second aspect of this project involves high-resolution synthesis and modeling of UV emissions based on recent laboratory measurements.

SCIENTIFIC OBJECTIVES

The scientific objectives are to develop a 2-D model, inversion codes and other computer tools needed to understand and use UV observations from space. These tools should be tested on real spacecraft observations. The second objective is to generate high-resolution synthetic spectra of O^2 for analysis of future observations.

APPROACH

We have and continue to develop, improve, and test accurate fast forward model sections. Additional codes are being produced to test and understand errors that arise from approximations and numeric methods. The forward model sections are then integrated into inversion drivers for the satellite UV observations. New methods use the 1-D inversion results to create the 2-D inversion results.

Data from the GLO experiment flown on the shuttle will be used to find both ionosphere and neutral densities in a multiple line inversion.

For the second primary objective, we are constructing line-by-line codes for the synthesis of molecular UV spectra in the lower ionosphere.

WORK COMPLETED

We have developed and verified fast and accurate programs to compute line of sight optical depths and intensities as observed by a spacecraft, including latitudinal variations. The first

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inversion algorithms for limb measurements that we developed in conjunction with NRL assumed a uniformly stratified atmosphere. The effects of latitude gradients were ignored. For many situations this is a good assumption, however often it will cause errors. We investigated the effect of latitude variations on inversions and found ionospheric errors in areas of steep gradients. We developed a 2D inversion and found improvements in the results.

GLO data obtained from the Space Shuttle has given us a nice data set to test inversion of multiple spectra data. The methods are working well. We are now using the limb profile of 9 lines to find ionospheric and atmospheric densities. This work is expected to be the Ph.D. thesis for my graduate student, Jin Wu. In addition we are continuing to improve our understanding of the complex numeric methods.

A line-by-line model of the oxygen Herzberg I bands has been constructed using recent FTS absorption measurements from the Harvard-Smithsonian Center for Astrophysics (Yoshino, et al., 1994). The measurements span the wavelength range 240-270 nm at 0.06 cm-1 resolution, and include rotationally-resolved absorption in the 4-0 to 11-0 vibrational bands. We have incorporated band oscillator strengths, A-state term values, and relative branch strengths from these measurements into our spectral model. Term values for the ground electronic state are based on previous determinations of X-state spectroscopic constants (Cheung, et al., 1996). The model contains tens line branches including vibrational levels v'=4-11 and v"=0-5, and rotational levels up to N"=23. Computations are done on a spectral grid of 0.05 cm^{-3} (the Doppler width at 295 K is approximately 0.09 cm-1). Calculated line shapes include a small pressure-broadening effect; results that follow assume a pressure of $10^{\wedge-3}$ mb.

The line-by-line synthesis compares favorably with the measurements by Yoshino, et al. (1994). A comparison between calculated and observed absorption is shown in Figure 1. The spectral region shown includes the 8-0 and 9-0 Herzberg I bands.

To simulate emission spectra, we have adopted absolute band strengths from the measurements by Hasson, et al. (1970). The strengths were originally derived by scaling relative values determined from emission (Degen and Nicholls, 1969) to the absolute value of the 7-0 band observed in absorption (Hasson and Nicholls, 1971). The more recent measurement of the 7-0 band strength from Yoshino, et al. (1994) is in excellent agreement (2%) with the Hasson and Nicholls result, and no rescaling has been applied to the relative band strengths. A preliminary estimate of the vibrational distribution of the A state is taken from the model results of Siskind and Sharp (1990) for intermediate quenching, which is based on the rocket measurements from Sharp and Siskind (1989). This distribution can alternately be retrieved from future measurements.

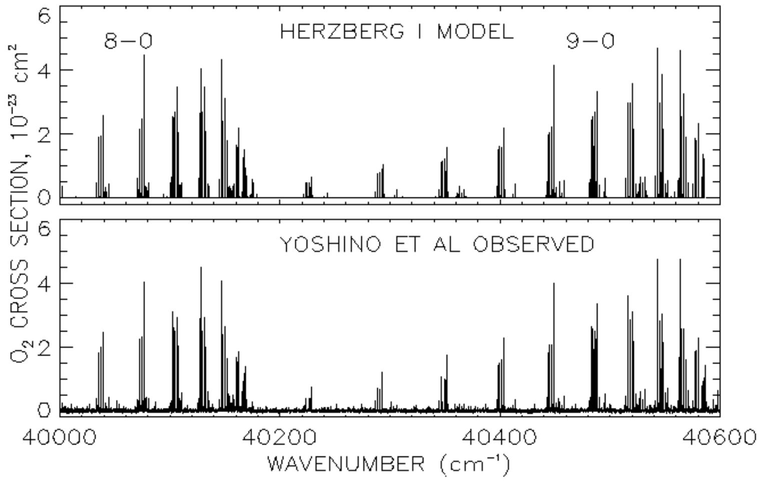

Figure 1. Herzberg I Absorption Cross Section for 8-0 and 9-0 Bands. Top Panel Shows Spectral Model, Bottom Panel from Measurements by Yoshino, et al, (1994).

RESULTS

Observations of 834 A intensities were simulated for an entire orbit. These observations were inverted in several ways. Figure 2 shows the results of these test inversions. The errors resulting from the 1-D and from the 2-D inversions are also shown. The error in the 2-D inversion are smaller.

Nine emission lines of GLO data have been used simultaneously to find both ionospheric and neutral densities.

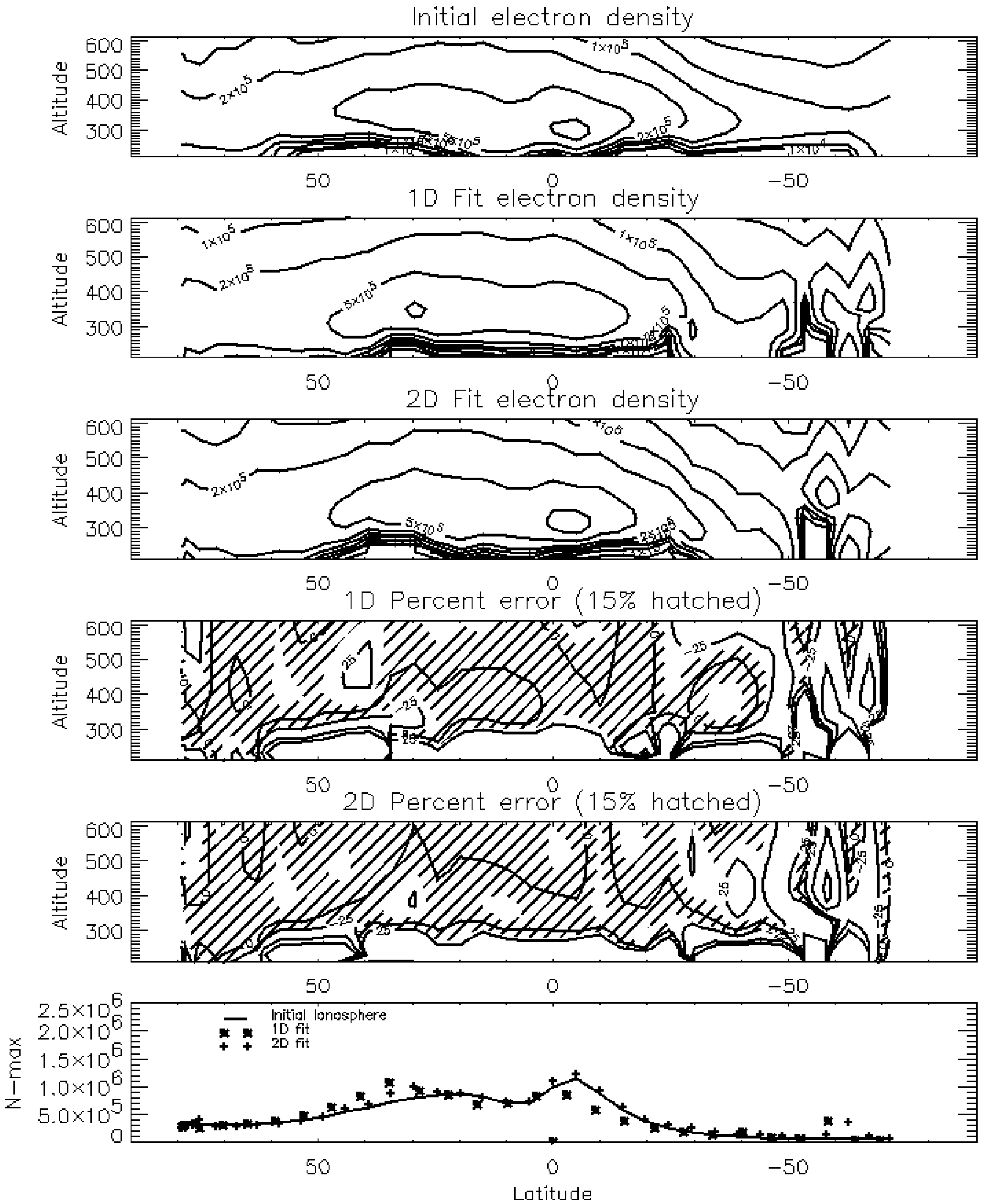

Figure 2. This Figure Indicates the Results of the 1D and 2D Inversions. The top panel is the actual electron density, the next two are the 1D and 2D fits. It can be seen the 2D fits better, but both do a poor job at the southern terminator.

The synthesis of the O2 spectra has led to several results. A comparison between the calculated column emission rate and the measurements presented by Siskind and Sharp is shown in Figure 3. The observed spectrum is a composite obtained from nighttime limb observations in the 90-95 km tangent height range. The calculated spectrum has been convolved with a slit function of 4 Angstroms FWHM (approximately the resolution of the measurements). Additionally, the measurements have been scaled to the model at the peak of the 6-2 band (2780 A) emission rate. This comparison indicates that measurements of this kind can be used with the model to constrain

O densities and vibrational distributions of the A state (e.g., Siskind and Sharp, 1990). However, the resolution is insufficient to reveal rotational structure for inferring temperature.

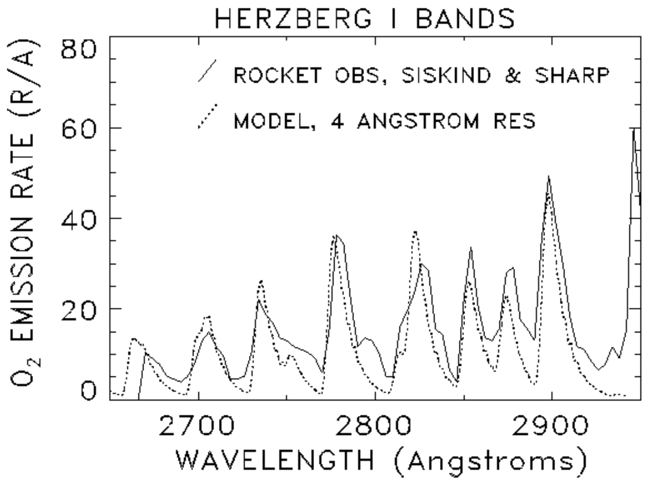

Figure 3. Oxygen Limb Emission Observed Near 90-95 km Tangent Height by Siskind and Sharp (1991) (solid curve), and Calculated Based on Herzberg I Emission (dotted).

A comparison to the ATLAS ISO measurements (Torr, et al., 1995) is shown in Figure 4. The measurements were obtained with a high resolution imaging spectrograph deployed from the space shuttle to observe the nighttime limb. At 2.3 A spectral resolution, rotational structure within each band becomes observable. Agreement between the model and observations is reasonably good, however there are discrepancies most likely related to the Herzberg II and III systems. Contributions to the emission from the Herzberg II system, first identified in the nightglow by Slanger and Huestis (1981), are absent from the synthetic spectrum but do appear in the nightglow, particularly since the Herzberg II band heads are well separated from those of the Herzberg I. Additionally, Sharp and Siskind (1989) identified the Herzberg III 6-2 band near 2815 A in their rocket measurements; inclusion of this band in the model might improve the agreement in this spectral region. Discrepancies between Herzberg I band heads are also affected by possible wavelength offsets (the ISO data appear shifted by ~1 A with respect to the model) as well as increased noise at lower emission levels.

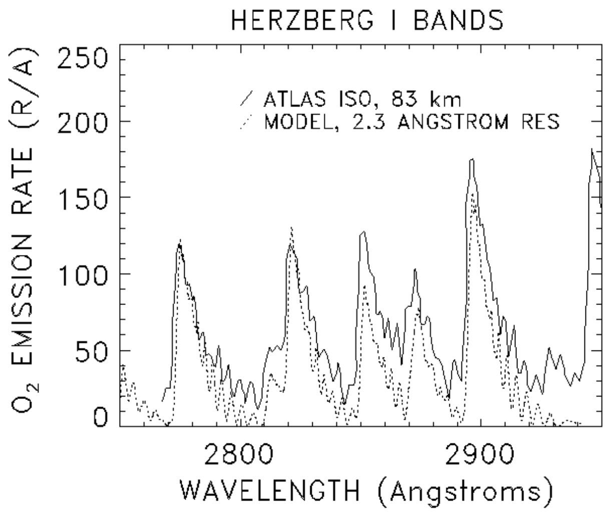

Figure 4. Oxygen Limb Emission Near 83 km Tangent Height Observed with the ISO Instrument (Torr, et al., 1995) (solid curve), and Synthetic Emission Spectrum (dotted).

Other discrepancies may also be significant, such as the model under-prediction of the peak intensity near 2850 A. The excess emission was tentatively attributed to the Mg I resonance line by Sharp and Siskind (1989). This issue warrants further investigation in future limb measurements of the nightglow.

IMPACT/APPLICATION

Improved techniques for ionosphere monitoring will lead to better models and predictions of electron and neutral densities.

RELATED PROJECTS

The inversion algorithms will be used to help interpret the measurements of the SSULI instruments (an NRL project). We have developed inversion algorithms in conjunction with NRL for a uniformly stratified atmosphere. Inversions the include the effects of latitude variation can also be used to find densities that effect the drag predictions of Robert Tolson. The inferred ionospheric densities will be comparison to the ionospheric models of Ray Roble.

We have the capability to accurately model spectral signatures in the O^2 Schumann-Runge and NO delta bands (e.g., Minschwaner and Siskind, 1993) which can be observed, for example, with the 1 A MUV spectrograph being developed by Bill McClintock at the University of Colorado. Additional progress, as noted above, is being made on the spectra of the oxygen Herzberg I bands.

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